TEFAL-2.2

Making ENDF-6 nuclear data libraries with TALYS

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About the author

Arjan Koning is a nuclear physicist with a Masters Degree in Theoretical physics at the Univ. of Amsterdam, a PhD in the Natural Sciences on Multi-step direct reactions at the Univ. of Groningen, and a Professorship at the Univ. of Uppsala on theoretical nuclear reactions.

Arjan is currently Head of the Nuclear Data Section at the IAEA in Vienna. Before that, he has worked at ECN/NRG Petten, the Netherlands, on nuclear reaction data for science and technology, and as guest scientist at CEA/Bruyères-le-Châtel and Los Alamos National Laboratory on the development and computational implementation of nuclear reaction models. He has led several students to PhD degrees, has coordinated and chaired various international nuclear data projects such as the OECD/NEA JEFF and WPEC projects, and has advised governments and international organisations on nuclear research and development. Among his scientific accomplishments are innovations in nuclear reaction physics, especially for the optical model and pre-equilibrium reactions, and initiating the '3 T's': the TALYS nuclear model code, Total Monte Carlo uncertainty propagation and the TENDL nuclear data library. He has been awarded the Oppenheimer Coin from Los Alamos National Laboratory, and the title of Doctor Honoris Causa by Uppsala University. As of 2025, his h-index is 62 with more than 26 000 citations.

Although Arjan is currently in a managerial role, he aims to keep his scientific creativity alive by maintaining and extending TALYS plus all software that emerges from that. Pleas from his friends to also spend time on other things are sometimes honoured.

Preface

TEFAL is a software package for the production of nuclear data libraries. Its main task is to process the output files of the TALYS nuclear reaction code, but also data from other sources such as resonance tables and other nuclear data libraries, into a data library in ENDF-6 format. After processing, these nuclear data libraries can be used in software such as Monte Carlo and deterministic reactor codes, transport and activation codes, for computational simulation of nuclear applications. The idea to make TEFAL was born in 2001, when TALYS was reaching some state of completeness and quality, and several of our projects required the production of nuclear data libraries. At that time, my knowledge of the ENDF-6 format was implemented in software to process the output of the GNASH code into ENDF-6 data files (this code, QUICKGNASH, was written during my stay in Los Alamos in the 90s, working with Phil Young and Mark Chadwick on their LA-150 library) and a code I wrote to produce and translate activation libraries (EAF2ENDF). These codes were dismantled, combined and reprogrammed into one single software package, TEFAL, which is getting close to becoming an implementation of the entire ENDF-6 formats manual. The objective of TEFAL is to provide a complete ENDF-6 formatted data library of user-dependent complexity and completeness, using data from any source, with TALYS as the main provider of data.

Like most scientific projects, TEFAL is always under development. Nevertheless, at certain moments in time, we freeze a well-defined version of TEFAL and subject it to extensive verification and validation procedures. You are now reading the tutorial of version 2.2.

License, contact and reference

As mentioned on the first page and in the source code, TEFAL falls in the category of MIT License software.

In addition to the MIT *terms* I have a *request*:
- When TEFAL is used for your reports, publications, etc., please make a proper reference to the code. At the moment this is:

A.J. Koning, D. Rochman, J.-Ch. Sublet, N. Dzysiuk, M. Fleming, and S. van der Marck, TENDL: Complete Nuclear Data Library for innovative Nuclear Science and Technology, Nuclear Data Sheets 155,1 (2019).

The webpage for TEFAL is **nds.iaea.org/talys**.

Acknowledgements

Arjan Koning

Contents

1. Introduction

TEFAL is a module for the translation of the nuclear reaction results of the nuclear model code TALYS [1], and information from other sources such as resonance tables and other nuclear data libraries, into ENDF-6 formatted nuclear data libraries. The basic objective behind the construction of TEFAL is to create nuclear data files without error-prone human interference. Hence, the idea is to run TALYS for a projectile-target combination and a range of incident energies, and to obtain a ready to use nuclear data library from the TEFAL code through processing of the TALYS results, possibly in combination with experimental data, resonance parameters, or data from existing data libraries. This procedure should be both systematic and automated, so that the probability of errors, coming from "manual" evaluation and editing of the datafile, is minimized. This "manual" evaluation, which is always present when there is experimental data, consists basically of implementing nuclide-specific knowledge in (nuclear model code) input files and scripts and should take place at the start of the library production chain.

The nuclear data libraries that are constructed with this method provide essential information for existing and new nuclear technologies. Important applications that rely directly or indirectly on data libraries generated by TALYS and TEFAL are conventional and advanced power reactors (GEN-IV), transmutation of radioactive waste, fusion reactors, homeland security, medical isotope production and radiotherapy, accelerator shielding, oil-well logging, and geophysics. Before this release, TEFAL has already been used for the above fields.

The following types of nuclear data library can be produced with the TALYS-TEFAL combination:

- Neutron general purpose libraries in ENDF-6 format, up to 20, 30, 200 MeV or any other incident energy within the TALYS domain,
- photonuclear general purpose libraries in ENDF-6 format,
- proton, deuteron, triton, Helium-3, and alpha general purpose libraries in ENDF-6 format, up to 200 MeV,
- Activation libraries up to any incident energy for all particles.

The above list may look somewhat fragmented, but we present it this way to allow various users to recognize the type of library they require. The whole list could be summarized as follows: General purpose and activation data libraries in ENDF-6 format, for any type of projectile, for energies up to 200 MeV, including covariance data, and with user-defined switches between different ENDF-6 procedures.

The precision and completeness requests made to the nuclear data evaluator are challenging enough, and ideally no time should be wasted with manual construction or updating parts of a nuclear data library. If the basic experimental and theoretical (computational) nuclear reaction information is well assessed, it is important that it reaches nuclear applications without any further approximations, omissions or formatting mistakes. It is thus important to have a code like TEFAL available. As specific features of TEFAL we mention

- Storage of cross sections, angular distributions, energy spectra, double-differential spectra, gamma-ray production, fission quantities, residual nuclide production (including isomers), and recoil information in ENDF-6 format.
- Flexibility to choose between different ENDF-6 options and procedures.
- Robustness, enabling the TALYS-TEFAL combination to be used in scripts that produce a huge number of data libraries, such as TENDL [2] and ensuring reproducibility of nuclear data libraries "from scratch".
- Automatic inclusion of resonance data from existing libraries or (preferably) from the TARES code [3].
- Automatic inclusion of specific types of data from other software, existing nuclear data libraries, for the cases which TALYS may not handle well enough, such as low energy total cross section data, the average number of fission neutrons (TAFIS code[2]) and the prompt neutron fission spectra (TANES code[2]), and finally data which can maybe be produced by TALYS, but which we think are better in other existing libraries.
- Formatting of covariance data by using the TASMAN-TALYS-TEFAL combination. TASMAN [2] is a code for Monte Carlo-based covariance methods, optimization to experimental data and sensitivity calculations.
- A transparent source program, validated using many compilers.
- Input/output communication that is easy to use and understand.
- A user manual.
- Several sample cases.

The central message is that we provide a complete nuclear data library of user-dependent complexity, directly from the results of TALYS or other software, like TARES, TAFIS and TANES, and, if requested, parts of existing data libraries. The first outline of the results of this combination was presented in Ref [4].

With TEFAL, a complete nuclear data library can already be obtained with minimal effort, namely by running it with a blank input file. This gives you a standard, though very complete, nuclear data library as the result. If you want to be more specific on ENDF formatting options, you simply add some of the more than 50 keywords that can be specified in TEFAL. Similar to TALYS, we thus do not ask you to understand the precise meaning of all these keywords in your first attempt: you can make your input file as simple or as complex as you want.

In this manual, we will give an outline of TEFAL as a stand-alone code, i.e. not necessarily as part of a large evaluation system Throughout this tutorial, sample cases are described.

1.1 How to use this tutorial

For evaluators that produce ENDF-6 nuclear data files, probably most of this manual is relevant, and you may check below whether parts can be skipped. After this Introduction, you will find

Chapter 2: Installation guide,

Chapter 3: Input description, a short description of the basic input rules.

Chapter 4: A description of the procedures used to create the ENDF-6 files including a description of the various MF and MT numbers. This Chapter also contains the sample cases.

Chapter 5: Reference guide with a description of all the keywords.

Chapter 6: Outlook and conclusions.

2. Installation and getting started

2.1 The TEFAL package

In what follows we assume TEFAL will be installed on a Linux or MacOS operating system. The total TEFAL package is in the *tefal/* directory and contains the following directories and files:

- *LICENSE* is the license file,
- *README.md* outlines the contents of the package,
- *install_tefal.bash*, *code_build.bash* and *path_change.bash* are scripts that take care of the installation,
- *source/* contains the Fortran source code of TEFAL,
- *bin/* contains the TEFAL binary after successful compilation,
- *misc/* contains miscellaneous files used by TEFAL or related scripts,
- *doc/* contains the documentation: this manual in pdf format.
- *samples/* contains the input and output files of the sample cases.

In total, you will need only a few tens of Mb of free disk space to install TEFAL. The code has so far been tested by us on various Linux and MacOs systems, so we can not guarantee that it works on all operating systems, although we know that some users have easily installed TEFAL under Windows. The only machine dependencies we can think of are the directory separators '/' we use in pathnames that are hardwired in the code. If there is any dependence on the operating system, the associated statements can be altered in the subroutine *machine.f90*. Also, the output of the execution time in *timer.f90* may be machine dependent. The rest of the code should work on any computer.

2.2 Installation

The installation of TEFAL is straightforward. You can download TEFAL via either git

- **git clone https://github.com/arjankoning1/tefal.git**

or by getting the tar file

- **https://nds.iaea.org/talys/tefal.tar**
- **tar zxf tefal.tar**

We here provide the necessary steps to do the installation, For a Linux or MacOs system, the installation is expected to be handled by the *install_tefal.bash* script, as follows

- if necessary, edit *code_build.bash* and set the first two variables: the name of your compiler and its flags.
- **install_tefal.bash**

An alternative installation option is

- **cd tefal/source**
- **make**

If this does not work for some reason, we here provide the necessary steps to do the installation manually. For a Linux or MacOS system, the following steps should be taken:

- **cd tefal/source**
- Ensure that TEFAL can read the binary directory with the TALYS and/or other executables. This is done in subroutine *machine.f90*. If *code_build* has not already replaced the path name in *machine.f90*, do it yourself. We think this is the only machine dependence of TEFAL. We expect no complaints from the compiler.
- **gfortran -c *.f90**
- **gfortran *.o -o tefal**
- **mv tefal ../bin**

The above commands represent the standard compilation options. Consult the manual of your compiler to get an enhanced performance with optimization flags enabled. We note that the part of a total run that is taken by TEFAL generally takes only takes a few seconds so extreme optimization is not necessary. It is the underlying TALYS run that may be time consuming.

2.3   Verification and sample cases

If TEFAL is installed, testing the sample cases is the logical next step. The *samples/* directory contains the script *verify* that runs all the test cases. Each sample case has its own subdirectory, which contains a subdirectory *org/*, where we stored the input files and **our** calculated results. It also contains a subdirectory *new/*, where we have stored the input files only and where the *verify* script will produce **your** output files. Of course, it is assumed that you have TALYS installed, see the TALYS manual, to do the underlying nuclear model calculations. A full description of the keywords used in the input files is given in Chapter 5. The sample cases are scattered throughout this tutorial. Note that in each subdirectory a file 'outputdiff' with differences with our original output is created.

2.4   Getting started

If you have created your own working directory with an input file named e.g. *tefal.inp*, then a TEFAL calculation can easily be started with:

talys < **talys.inp** > **talys.out**

tefal < **tefal.inp** > **tefal.out**

where the name *tefal.inp* is not obligatory: you can use any name for this file. Besides the general output file *tefal.out* various other output files are produced with the ENDF-6 file as the most important one. Of course, a TALYS calculation with keyword **endf y** is required first.

3. Input description

For people who want to go straight to work and will not wait for sample cases later in this tutorial, we give the most important input rules here. For the communication between TEFAL and its users, we have constructed an input/output method which shields beginners from all the possible options for parameters that can be specified in TEFAL, while enabling at the same time maximal flexibility for experienced users. The rules are basically the same as those for TALYS.

An input file of TEFAL consists of keywords and their associated values. We have devoted the entire chapter 5 of this tutorial to the input possibilities with the Reference Guide, but let us illustrate the use of the input by an example. We note here that the minimum input file for TEFAL is a blank file, i.e. on a Linux system a simple **touch tefal.inp** followed by **tefal < tefal.inp > tefal.out** will suffice, *provided you have first done a TALYS run with keyword* **endf y** *in the TALYS input file*. The blank TEFAL input file represents the simplest possible job for TEFAL: make an ENDF-6 data file. Behind this simple input file, however, there are about 50 default values that TEFAL uses for the various parameters, procedures for specific MF/MT combinations, names of output files, level of detail, etc, that you may want to alter. When you use the minimal blank input file, you leave it to the author of TEFAL to choose all the parameters for you, as well as the level of detail of the ENDF-6 file. If you want to use specific parameters or want to have more, or less, specific information in the data file, you will have to enter more keywords, such as in this example:

```
partiald y
Eswitch              30.
adopt 3 1 n-Co59.jeff3.3 1.e5 7.e5
```

In this chapter, we will just give the basic rules that must be obeyed when constructing an input file for TEFAL. Next, an outline of all the keywords is given in Chapter 5.

3.1 Basic input rules

Theoretically, it would be possible to make the use of TEFAL completely idiot-proof, i.e. to prevent the user from any input mistakes that possibly can be made and to continue a calculation with "assumed" values. Although we have invested a relatively large effort in the user-friendliness of TEFAL, we have not taken such safety measures to the extreme limit and ask at least some minimal responsibility from the user. Once you have accepted that, only very little effort is required to work with the code. The input rules are basically equal to those of TALYS. Successful execution of TEFAL can be expected if you stick to the following simple rules and possibilities of the input file:

1. One input line contains one keyword. Usually it is accompanied by only one value, but some keywords (e.g. **adopt**) need to be accompanied by more than one value on the same line.
2. A keyword and its value(s) *must* be separated by at least 1 blank character.
3. The keywords can be given in arbitrary order. If you use the same keyword more than once, the value of the last one in the input file will be adopted.
4. All characters can be given in either lowercase or uppercase.
5. A keyword *must* be accompanied by a value. To use default values, the keywords should simply be left out of the input file.
6. An input line starting with a # in column 1 is neglected. This is helpful for including comments in the input file or to temporarily deactivate keywords.
7. TEFAL only works after a TALYS run, with the keyword **endf y** specified in the TALYS input file.

As an example of rules 3, 4, and 6, it can be seen that the following input file is completely equivalent to the one given in the beginning of this chapter:

```
# Equivalent input file
partiald y
Eswitch              30.
adopt 3 1 n-Co59.jeff3.3 1.e5 7.e5
#gpf n
```

In the following erroneous input file, only the second and fourth lines are correct, while rules 2, and 5 are violated in the other lines.

```
recoil
partiald y
Eswitch30.
adopt 3 1 n-Co59.jeff3.3 1.e5 7.e5
```

In cases like this, TEFAL will give a specific error message for the first encountered problem and the execution will be stopped. We like to believe that we have covered all such cases and that it is impossible to let TEFAL crash (at least with our compilers) without giving an appropriate error message, but you are of course invited to let us know about the contrary (Sorry, no cash rewards). Typing errors in the input file should be spotted by TEFAL, e.g. if you write **Eswwitch 30.**, it will tell you the keyword is not in our list, and the code will gracefully stop.

As explained above, the minimum input file is a blank file, i.e. to leave all choices for ENDF-6 procedures to the author. In general, you probably want to be more specific. In Chapter 5, we will explain all the possible keywords. We have classified them according to their meaning and importance. For each keyword, we give an explanation, a few examples, the default value, and the theoretically allowed numerical range. Remember that you can always find all adopted default values for all parameters at the top of the standard *output* file of TEFAL.

4. Nuclear data files in ENDF-6 format

The data files which are created with TEFAL are generally a combination of output results from TALYS, data from other software and existing data tables or libraries. Non-TALYS data are usually neutron resonance data, low-energy neutron total, elastic, capture or fission cross sections, average number of fission neutrons, and fission neutron spectra, but other parts of existing libraries can be added too. The combination of this is processed into an ENDF-6 file. The full ENDF-6 format for storing nuclear data is documented in the ENDF-6 manual [5]. Here, we restrict ourselves to those ENDF-6 procedures that we find the most appropriate for the production of modern, complete and processable nuclear data libraries. As outlined in Ref. [5]. classes of quantities such as cross sections, angular distributions, covariance data, etc. are represented by so-called MF-numbers, whereas different reaction channels such as (n,tot), (n,2n), etc. are represented by MT-numbers. Together, the MF/MT combinations allow for a complete representation of a nuclear reaction. For every reaction channel TEFAL writes all cross sections, energy spectra, angular distributions, associated photon production, etc. that are provided by TALYS, or other sources, to the appropriate MF/MT section in the ENDF-6 format.

Most effort of both TALYS and TEFAL has gone into the simulation and formatting of low energy neutron data, not only because this is the most important energy range for most of our customers, but this is also the energy region where both nuclear modeling and data formatting is the most complicated. However, one difference with many traditional nuclear data libraries is that TEFAL can produce data files that extend up to 200 MeV (or higher if data are available), and also for incident particles other than neutrons, provided of course that such data have been calculated with TALYS first.

We will first give a description of each MF section, and the various options that have been programmed into TEFAL to fill these sections, first for the central values and then for covariance data. In principle, this outline is always done with incident neutrons in mind, but we will make special mention for incident photons and charged particles, when appropriate. After that, we discuss

two standard procedures to make a complete ENDF-6 file which gives the most specific information and flexibility in use. The user may deviate from the standard procedures by setting the various keywords that are explained in chapter 3. Again, a complete description of all the options to store data can be found in the ENDF manual [5].

Sample case 4.1 **20 MeV neutron general purpose file for ^{72}Ge**
This sample case concerns a conventional neutron data library, i.e. a general purpose library up to an energy of 20 MeV for ^{72}Ge. A total of 4 files are needed for this run: the TALYS input file *talys.inp*, the energy grid *energies*, the optical model file *ge.omp* that is specified in the TALYS input file (for this particular case, see input file below) and the TEFAL input file *tefal.inp*. First, a TALYS calculation is performed

talys $<$ talys.inp $>$ talys.out

where the input file *talys.inp* looks as follows:

```
#
# General
#
projectile n
element ge
mass 72
energy energies
endf y
#
# Precision
#
bins 40
popeps 1.e-12
transeps 1.e-20
transpower 15
xseps 1.e-30
#
# Specific
#
M2constant 1.2
Rgamma 3.
a 30 69 10.0
Ntop 30 73 15
a 30 73 12.9
a 31 70 12.0
a 31 72 12.7
Ntop 31 73 15
a 31 73 12.6
a 31 74 12.0
a 32 69 12.5
```

```
a 32 70 12.0
a 32 71 10.8
a 32 72 11.1
a 32 74 10.8
a 32 76 11.0
gp 32 73 2.7
optmodfileN 32 ge.omp
```

Note the essential input line with **endf y**. For the rest, the TALYS input consists of some adjustable nuclear model parameters and some parameters determining the precision. We refer to the TALYS manual for the exact meaning of these keywords. The TEFAL input file is empty for this sample case, though needs to exist. TEFAL is executed

tefal < tefal.inp > tefal.out

After this run, the most important result is a file called *n-Ge072.gpf*, which is the complete ENDF-6 formatted file. The top of this file shows the well-known ENDF format:

```
TENDL-2023 gen. purp. file: neutron  + Ge- 72  1.e-5 eV -  20 MeV  99 0  0     0
3.207200+4 7.130424+1           1         0        17        13231 1451    1
0.000000+0 0.000000+0           0         0         0        63231 1451    2
1.000000+0 2.000000+7           1         0        10     20233231 1451    3
0.000000+0 0.000000+0           0         0       377      1633231 1451    4
32-Ge- 72 IAEA       EVAL-DEC23 A.J. Koning and D. Rochman      3231 1451    5
TENDL-2023          DIST-     REV1-                             3231 1451    6
----TENDL-2023      Material 3231          REVISION 1           3231 1451    7
-----Incident neutron  data                                    3231 1451    8
------ENDF-6 Format                                            3231 1451    9
```

In addition, there is the standard TEFAL output file *tefal.out* which looks as follows

```
   TEFAL-2.2 (Version: December 9, 2025)


         Creating ENDF-6 files with TALYS


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 ########### DATA FILE ##########


 TENDL-2025: neutron  + Ge- 72  1.e-5 eV -  20 MeV       CC-BY-4.0


 ########## USER INPUT ##########


 USER INPUT FILE
```

```
adopt 2 151 n-Ge072.mf2

USER INPUT FILE + DEFAULTS

Keyword          Value   Variable      Explanation

#
# Type of data library
#
gpf               y      flaggpf       flag for general purpose library
eaf               n      flageaf       flag for EAF-formatted activation libra
#
# Specific structure of the data file
#
linenumbers       y      flaglinenum   flag to write line numbers of ENDF file
high              n      flaghigh      flag for high energies
mtall             y      flagmtall     flag to include all defined MT numbers
mtextra           n      flagmtextra   flag to include extra numbers up to MT2
Eswitch         30.000   Eswitch       energy where ENDF-6 representation is s
Eswitch4        30.000   Eswitch4      energy where MF4 representation is swit
cuteps           0.000   cuteps        energy shift  at MT5 cutoff energy (in
resonance         y      flagres       flag to include resonance parameters
capt6             y      flagcapt6     flag to put all MT102 gamma production
disc6             n      flagdisc6     flag to put all discrete angular distri
part6             y      flagpart6     flag to put all gamma production for pa
rp6               y      flagrp6       flag to put all residual production cro
rp10              n      flagrp10      flag to put all residual production cro
fis10             n      flagfis10     flag to put (subactinide) fission cross
gam13             n      flaggam13     flag to use MF13 for gamma production i
gamdisc           y      flaggamdisc   flag to store gamma production per disc
gamspectrum       n      flaggamspec   flag to store gamma production only as
ngn               n      flagngn       flag to include (n,gamma n) data
partialn          y      flagparn      flag to include partial cross sections
partialp          n      flagparp      flag to include partial cross sections
partiald          n      flagpard      flag to include partial cross sections
partialt          n      flagpart      flag to include partial cross sections
partialh          n      flagparh      flag to include partial cross sections
partiala          n      flagpara      flag to include partial cross sections
endfdetail        y      flagendfdet   flag for detailed ENDF-6 information pe
addlow            y      flagaddlow    flag to add low-energy Q>0 reactions to
clean             y      flagclean     flag for cleaning up double points
renorm            y      flagrenorm    flag for renormalization of spectra
multichance       y      flagmulti     flag to include multi-chance fission
recoil            n      flagrecoil    flag to include recoil information
subfission        n      flagsubfis    flag to include subactinide fission
```

```
urrmode              0     urrmode      0: no URR, 1: URR from TALYS, 2: URR fr
lssf                -1     lssfinp      0: URR cross section from MF2, 1: URR c
urrcomp              1     urrcomp      mode for competition in the URR, 0:none
urrenergy     -1.00000 urrenergy      upper energy of the URR in MeV
NMTmax             400 NMTmax          maximum number of MT numbers
disclim          10.00 disclim         limit for specific MT numbers for discr
tabddx               n     flagtabddx   flag to give explicit DDX in MF6
#
# Use of specific data
#
adopt      2 151 n-Ge072.mf2 1.00000E-05 2.00000E+08
#
# Information for MF1
#
author              A.J. Koning and D. Rochman
lab                 IAEA
identifier          TENDL-2025
endftext            /Users/koning/tefal/misc/endf_n.txt
#
# Covariance data
#
covariance           n     flagcovar    flag for covariances
partialcov           n     flagparcov   flag to include covariances for MT600-8
covdiscrete          4     covdiscrete  number of discrete inelastic levels wit
intercor             y     flagintercor flag for inter-MT covariance data
#
# Miscellaneous
#
endffile n-Ge072.gpf endffile      name of ENDF file


Number of deleted points:    55 (see file tefal.clean)


Execution time:  0 hours  0 minutes 10.57 seconds


TEFAL has created the following ENDF-6 file: n-Ge072.gpf
```

Note that a table with all keywords is given, not only the ones that you have specified in the input file (in this case: none), but also all the defaults that are set automatically. The corresponding Fortran variables are also printed, together with a short explanation of their meaning. This table can be helpful as a guide to change further input parameters for a next run. Finally, at the end of the output it is mentioned that a file *tefal.clean* is made which contains a list of cleaned up double points.

The ENDF file of this sample case shows the default ENDF-6 procedures we have used (since *tefal.inp* is empty): all open channels are included (many MT numbers), inelastic scattering

angular distributions for discrete levels are stored in MF4/MT51, etc, MF6 is used for secondary distributions of partial channels, and MF12 is used for discrete level photon production.   ■

4.1   ENDF-6 data file procedures covered by TEFAL

As mentioned, we describe below the possibilities that have been implemented in TEFAL. This may be regarded as a first "filtering" action on the ENDF manual, leaving only the procedures that should survive in modern evaluations. We realize that this is subjective, but we think that the combination of procedures we have chosen is the most robust for the various processing codes. It becomes even more subjective when we summarize our "preferred" procedure to obtain complete, processable data files in section 4.3.

Depending on the projectile, purpose, and type of library, each evaluated file may contain the following data.

4.1.1   MF1: General information

Each data file starts with the usual header information like author, type of library, maximum energy, name of institute, etc. Next, a textual description of the evaluation methods, experimental data used, etc. is included. Also, the full directory of used MF/MT sections is given.

In neutron libraries for actinides, MF1 also contains the average number of neutrons from fission. In the current version of TEFAL, these are adopted from existing data libraries or, if not available, from systematics. The best combination of these two sources is often sorted out by the TAFIS code[2], whose output can be directly used by TEFAL. The total number of neutrons is given in MT452, the delayed neutron data in MT455 and the prompt neutron data in MT456. The components of energy release from fission are given in MT458. The **adopt** keyword is available to choose between various sources (existing libraries or systematics) for these data.

4.1.2   MF2: Resonance parameters

MF2 is only used, and allowed, for incident neutrons. Resonance parameters are adopted from the best possible data set, where "best" denotes a combination of most recent and completeness of the resonances. In the majority of cases, MF2 is generated by the TARES code[3], which extracts resonance parameters from the latest measurements (as obtained from the EXFOR database), from compilations (*i.e.* The Atlas of Neutron Resonances [6]), or existing data libraries and turns that into ENDF-6 format. TARES thus produces the best set of resonance parameters per nucleus, an admittedly subjective choice, which also forms the basis of TENDL [2]. The first two of these sources of information cover the vast majority of experimental data used in TEFAL. The data are generally stored in Reich-Moore format for non-actinides and Multi-Level Breit-Wigner format for actinides. As the source for resonance parameters is a subjective choice, it can easily be overruled by the user with the **adopt** keyword. In case of adoption of resonance data from other libraries, TEFAL also "beautifies" the resonance data, i.e. all data is rewritten using the e11.6 format, without leading zeroes or leading blanks etc. Resonance parameters are given for both the RRR and URR.

4.1.3   MF3: Reaction cross sections

By default, all cross section data come from TALYS, while sometimes we also take a small part of the data from other sources. TALYS stores all calculated data in separate output files which TEFAL then writes to separate MT-sections of MF3. The correspondence between these two sets is given in Tables 4.1-4.1.3. A summarized classification of these cross sections is as follows:

- Total (MT1), elastic (MT2) and non-elastic (MT3) cross sections.
- Inelastic cross sections to discrete states (MT51-90) and other binary cross sections for discrete levels such as (n,p) (MT600-640).
- Continuum inelastic cross sections (MT91) and other continuum cross sections such as (n,p) (MT649).
- Exclusive channel cross sections, e.g. (n,γ) (MT102), (n,n') (MT4), (n,2n) (MT16), (n,p) (MT103), (n,nα) (MT22), etc.
- For fissionable nuclides, fission cross sections (MT18-21,38)

If the user requests so, a complete description of all open channels (and associated MT-numbers) is included, provided the maximum cross section in an excitation function over the whole energy range exceeds 1.e-9 b. In each MT section, enough incident energies are used to provide a realistic representation of the energy-dependent cross sections.

In general, the elastic scattering cross section is obtained by subtracting the non-elastic cross section from the total cross section. If low energy cross sections are adopted from an existing data library or experiment, the elastic cross section is thus derived from evaluated, usually experiment-based, total cross sections and optical model based non-elastic cross sections. All experimentally observed structure in the data, which would not be predicted by an optical model, is thus automatically retained.

High-energy cross sections

For the construction of a high energy data file, say up to 200 MeV, procedures different from those used in the low energy files have to be employed, since it is no longer possible to store all reactions that describe different sequential particle emissions in separate MT-numbers. There are two possibilities to solve this. The first is to keep the detailed representation of neutron cross sections into several MT sections below 20 MeV, and after the introduction of new MT numbers in 2010 a limit of 60 MeV is now also proposed. In TEFAL, with the **Eswitch** keyword the switching energy may be chosen. Next, we one can switch to a more lumped description above 20 or 60 MeV [7, 8, 9, 10]. Most high-energy libraries, as in e.g. ENDF/B-VIII and TENDL, follow this procedure. For energies above 20(60) MeV, MT5 then contains the total non-elastic cross section, i.e. it is equal to MT3. By itself, this quantity is not very interesting, since it is too inclusive, i.e. it comprises all the partial cross sections. It can however be combined with the particle yields and relative energy-angle distributions of MF6/MT5 to obtain the particle production cross sections and double-differential cross sections. The total non-elastic cross section thus serves as an important normalization of all the non-elastic partial processes that take place. Of course, one would have to make sure that the actual cross section excitation curves remain continuous at 20(60) MeV after reconstruction. For example, the (n,2n) cross section is given in MT16 up to 20(60) MeV and as a residual production yield, for the nuclide reached after an (n,2n) reaction, in MF6/MT5. At 20(60) MeV, the same cross section value should emerge at these two different locations.

It is also possible to adopt a different procedure, in which there is no abrupt switch at 20(60) MeV. Instead, the MT sections which are used at low energies are used all the way up to the upper energy, e.g. 200 MeV, of the data file, and MT5 is only used for the *remaining* cross section. i.e. the sum of cross sections which are not stored in the MT numbers for exclusive reactions. The cross section in MT5 thus gradually increases with energy as more channels can not be represented by a pre-defined MT number. This has the advantage that the cross sections for a particular reaction channel remain inside one and the same MT number. Also, it is possible to make use of more exclusive secondary information, such as covariance information in MF33 up to 200 MeV, instead of giving this information only up to 20(60) MeV. A difficulty in creating such data files is that at

Table 4.1: The ENDF-6 MT numbers that can be considered in TEFAL and the corresponding TALYS output files.

MT	Reaction	MF3 (TALYS)	MF4,6 (TALYS)
1=2+3	total	total.tot	
2	elastic	elastic.tot	nnxxx.xxxleg.L00
3=4+5+[11-18]+[22-37] +[41-45]+[102-117]	non-elastic	nonelastic.tot	
4=[51-90]+91	total (n,n')	xs100000.tot	
5	(n,x)		
11	(n,2nd)	xs201000.tot	sp201000Exxx.xxx.tot
16	(n,2n)	xs200000.tot	sp200000Exxx.xxx.tot
17	(n,3n)	xs300000.tot	sp300000Exxx.xxx.tot
18=[19-21]+38	total (n,f)	fission.tot	
19	1st-chance (n,f)	xs000000.fis	
20	2nd-chance (n,f)	xs100000.fis	
21	3rd-chance (n,f)	xs200000.fis	
22	(n,nα)	xs100001.tot	sp100001Exxx.xxx.tot
23	(n,n3α)	xs100003.tot	sp100003Exxx.xxx.tot
24	(n,2nα)	xs200001.tot	sp200001Exxx.xxx.tot
25	(n,3nα)	xs300001.tot	sp300001Exxx.xxx.tot
28	(n,np)	xs110000.tot	sp110000Exxx.xxx.tot
29	(n,n2α)	xs100002.tot	sp100002Exxx.xxx.tot
30	(n,2n2α)	xs200002.tot	sp200002Exxx.xxx.tot
32	(n,nd)	xs101000.tot	sp101000Exxx.xxx.tot
33	(n,nt)	xs100100.tot	sp100100Exxx.xxx.to
34	(n,nh)	xs100010.tot	sp100010Exxx.xxx.tot
35	(n,nd2α)	xs101002.tot	sp101002Exxx.xxx.tot
36	(n,nt2α)	xs100102.tot	sp100102Exxx.xxx.tot
37	(n,4n)	xs400000.tot	sp400000Exxx.xxx.tot
38	4th-chance (n,f)	xs300000.fis	
41	(n,2np)	xs210000.tot	sp210000Exxx.xxx.tot
42	(n,3np)	xs310000.tot	sp310000Exxx.xxx.tot
44	(n,n2p)	xs120000.tot	sp120000Exxx.xxx.tot
45	(n,npα)	xs110001.tot	sp110001Exxx.xxx.tot
51-90	(n,n'$_1$) - (n,n'$_{40}$)	nn.L01-nn.L40	nnxxx.xxxleg[ang].L01-L40
91	continuum (n,n')	nn.con	sp100000Exxx.xxx.tot
102	(n,γ)	xs000000.tot	sp000000Exxx.xxx.tot
103=[600-649]	(n,p)	xs010000.tot	sp010000Exxx.xxx.tot
104=[650-699]	(n,d)	xs001000.tot	sp001000Exxx.xxx.tot

Table 4.2: The ENDF-6 MT numbers that can be considered in TEFAL and the corresponding
TALYS output files (continued).

MT	Reaction	MF3 (TALYS)	MF4,6 (TALYS)
105=[700-749]	(n,t)	xs000100.tot	sp000100Exxx.xxx.tot
106=[750-799]	(n,h)	xs000010.tot	sp000010Exxx.xxx.tot
107=[800-849]	(n,α)	xs000001.tot	sp000001Exxx.xxx.tot
108	(n,2α)	xs000002.tot	sp000002Exxx.xxx.tot
109	(n,3α)	xs000003.tot	sp000003Exxx.xxx.tot
111	(n,2p)	xs020000.tot	sp020000Exxx.xxx.tot
112	(n,pα)	xs010001.tot	sp010001Exxx.xxx.tot
113	(n,t2α)	xs000102.tot	sp000102Exxx.xxx.tot
114	(n,d2α)	xs001002.tot	sp001002Exxx.xxx.tot
115	(n,pd)	xs011000.tot	sp011000Exxx.xxx.tot
116	(n,pt)	xs010100.tot	sp010100Exxx.xxx.tot
117	(n,dα)	xs001001.tot	sp001001Exxx.xxx.tot
152	(n,5n)	xs500000.tot	sp500000Exxx.xxx.tot
153	(n,6n)	xs600000.tot	sp600000Exxx.xxx.tot
154	(n,2nt)	xs200100.tot	sp200100Exxx.xxx.tot
155	(n,tα)	xs000101.tot	sp000101Exxx.xxx.tot
156	(n,4np)	xs410000.tot	sp410000Exxx.xxx.tot
157	(n,3nd)	xs301000.tot	sp301000Exxx.xxx.tot
158	(n,ndα)	xs101001.tot	sp101001Exxx.xxx.tot
159	(n,2npα)	xs210001.tot	sp210001Exxx.xxx.tot
160	(n,7n)	xs700000.tot	sp700000Exxx.xxx.tot
161	(n,8n)	xs800000.tot	sp800000Exxx.xxx.tot
162	(n,5np)	xs510000.tot	sp510000Exxx.xxx.tot
163	(n,6np)	xs610000.tot	sp610000Exxx.xxx.tot
164	(n,7np)	xs710000.tot	sp710000Exxx.xxx.tot
165	(n,4nα)	xs400001.tot	sp400001Exxx.xxx.tot
166	(n,5nα)	xs500001.tot	sp500001Exxx.xxx.tot
167	(n,6nα)	xs600001.tot	sp600001Exxx.xxx.tot
168	(n,7nα)	xs700001.tot	sp700001Exxx.xxx.tot
169	(n,4nd)	xs401000.tot	sp401000Exxx.xxx.tot
170	(n,5nd)	xs501000.tot	sp501000Exxx.xxx.tot
171	(n,6nd)	xs601000.tot	sp601000Exxx.xxx.tot
172	(n,3nt)	xs300100.tot	sp300100Exxx.xxx.tot
173	(n,4nt)	xs400100.tot	sp400100Exxx.xxx.tot
174	(n,5nt)	xs500100.tot	sp500100Exxx.xxx.tot
175	(n,6nt)	xs600100.tot	sp600100Exxx.xxx.tot

Table 4.3: The ENDF-6 MT numbers that can be considered in TEFAL and the corresponding TALYS output files (continued).

MT	Reaction	MF3 (TALYS)	MF4,6 (TALYS)
176	(n,2nh)	xs200010.tot	sp200010Exxx.xxx.tot
177	(n,3nh)	xs300010.tot	sp300010Exxx.xxx.tot
178	(n,4nh)	xs400010.tot	sp400010Exxx.xxx.tot
179	(n,3n2p)	xs320000.tot	sp320000Exxx.xxx.tot
180	(n,3n2α)	xs300002.tot	sp300002Exxx.xxx.tot
181	(n,3npα)	xs310001.tot	sp310001Exxx.xxx.tot
182	(n,dt)	xs001100.tot	sp001100Exxx.xxx.tot
183	(n,npd)	xs111000.tot	sp111000Exxx.xxx.tot
184	(n,npt)	xs110100.tot	sp110100Exxx.xxx.tot
185	(n,ndt)	xs101100.tot	sp101100Exxx.xxx.tot
186	(n,nph)	xs110010.tot	sp110010Exxx.xxx.tot
187	(n,ndh)	xs101010.tot	sp101010Exxx.xxx.tot
188	(n,nth)	xs100110.tot	sp100110Exxx.xxx.tot
189	(n,nhα)	xs100011.tot	sp100011Exxx.xxx.tot
190	(n,2n2p)	xs220000.tot	sp220000Exxx.xxx.tot
191	(n,ph)	xs010010.tot	sp010010Exxx.xxx.tot
192	(n,dh)	xs001010.tot	sp001010Exxx.xxx.tot
193	(n,hα)	xs000011.tot	sp000011Exxx.xxx.tot
194	(n,4n2p)	xs420000.tot	sp420000Exxx.xxx.tot
195	(n,4n2α)	xs400002.tot	sp400002Exxx.xxx.tot
196	(n,4npα)	xs410001.tot	sp410001Exxx.xxx.tot
197	(n,3p)	xs030000.tot	sp030000Exxx.xxx.tot
198	(n,n3p)	xs130000.tot	sp130000Exxx.xxx.tot
199	(n,3n2pα)	xs320001.tot	sp320001Exxx.xxx.tot
200	(n,5n2p)	xs520000.tot	sp520000Exxx.xxx.tot
600-640	(n,p$_0$) - (n,p$_{40}$)	np.L00-np.L40	npxxx.xxxleg[ang].L01-L40
649	continuum (n,p)	np.con	sp010000Exxx.xxx.tot
650-690	(n,d$_0$) - (n,d$_{40}$)	nd.L00-nd.L40	ndxxx.xxxleg[ang].L01-L40
699	continuum (n,d)	nd.con	sp001000Exxx.xxx.tot
700-740	(n,t$_0$) - (n,t$_{40}$)	nt.L00-nt.L40	ntxxx.xxxleg[ang].L01-L40
749	continuum (n,t)	nt.con	sp000100Exxx.xxx.tot
750-790	(n,h$_0$) - (n,h$_{40}$)	nh.L00-nh.L40	nhxxx.xxxleg[ang].L01-L40
799	continuum (n,h)	nh.con	sp000010Exxx.xxx.tot
800-840	(n,α_0) - (n,α_{40})	na.L00-na.L40	naxxx.xxxleg[ang].L01-L40
849	continuum (n,α)	na.con	sp000001Exxx.xxx.tot

higher energies the lumped particle production yields and spectra of MF6/MT5 need to be corrected for the channels that have been taken into account explicitly in the other MT sections. This is challenging from a numerical point of view.

Sample case 4.2 **200 MeV neutron general purpose file for ^{45}Sc**

This sample case concerns a neutron data library up to an energy of 200 MeV, and leads to the ^{45}Sc evaluation as present in JEFF-3.1.

First, a TALYS calculation is performed

talys $<$ talys.inp $>$ talys.out

where the input file *talys.inp* looks as follows:

```
#
# General
#
projectile n
element sc
mass 45
energy energies
endf y
#
# Precision
#
bins 50
popeps 1.e-12
transeps 1.e-20
transpower 15
xseps 1.e-30
#
# Specific
#
spherical y
maxlevelsres 20
sysreaction d t h
M2constant 0.7
a 18 41 8.6
a 19 40 5.2
a 19 44 6.2
a 20 44 6.6
a 20 45 6.10
Ntop 21 45 30
Rgamma 3.
```

This time, the TEFAL input file *tefal.inp* is not empty, but we ask for adoption of the ENDF/B-VII total cross sections between 101 keV and 8.8 MeV, and the resonance parameters

from JENDL5.0. Moreover, we want to call our ENDF-6 file *Sc45.high*. The following input file is used

```
#
# General
#
endffile Sc45.high
#
# Adoption of data from other libraries
#
adopt 2 151 n-Sc045.jendl5.0
adopt 3 1 n-Sc045.endfb8.0 1.01e5 8.8e6
```

with which we run TEFAL
tefal < **tefal.inp** > **tefal.out**

For the same sample case we add an alternative input file which produces a different library *Sc45.alt*, namely one where there is no abrupt switch at 20 MeV, but where instead al MT numbers are filled with data up to 200 MeV. The file *tefal2.inp* that takes care of this looks as follows:

```
#
# General
#
endffile Sc45.alt
Eswitch 210.
mtall n
#
# Adoption of data from other libraries
#
adopt 2 151 n-Sc045.jendl4.0
adopt 3 1 n-Sc045.endfb8.0 1.01e5 8.8e6
```

with which we can also run TEFAL
tefal < **tefal2.inp** > **tefal2.out**

to produce the *Sc45.alt* file.

Charged-particle data

For incident charged particles, in principle the same possibilities exist to store data. There are however a few deviations from the neutron case. First of all the total cross section (MT1) is undefined, since it is infinite. This is a result of the charged-particle elastic scattering cross section which is the square of the sum of a nuclear amplitude and a Coulomb amplitude. This means that the charged-particle elastic scattering cross section is infinite since the associated angular distribution is dominated by the Rutherford formula for Coulomb scattering, which diverges at zero degrees. The ENDF-6 format allows to circumvent this and to store only the nuclear and the

Coulomb-nuclear interference cross section in MT2, so that it can be recombined with the Coulomb term afterwards. This quantity is obtained by integrating the associated angular distributions. Note that because of the interference effect, the tabulated values can be negative at some energies.

In most proton, or other charged-particle, evaluations the only other section in MF3 is MT5, which contains the total non-elastic cross section, with which the information of MF6/MT5 can be combined to obtain particle production cross sections and (double-)differential cross sections, similar to neutrons. It is however also possible to use specific MT numbers as for neutrons. In that case it is easier to read directly e.g. the (p,2n) cross section from MT16, instead of deriving it from the MF3-MF6/MT5 combination. There are indications however, that the processing route for this option is not (yet) stable enough. Hence, for applied calculations we often use the lumped presentation.

Sample case 4.3 **200 MeV proton general purpose file for ^{27}Al**

This sample case concerns a high-energy proton data library, i.e. up to an energy of 200 MeV. This time, no attempt was made to adjust the TALYS results to experimental data. This is a so called "blind" data library. The following TALYS input file is used:

```
#
# General
#
projectile p
element al
mass 27
energy energies
endf y
```

with which we run
talys $<$ talys.inp $>$ talys.out

while *tefal.inp* is empty, so that running
tefal $<$ tefal.inp $>$ tefal.out

produces the file *p-Al027.gpf*.   ■

Photonuclear data

For incident photons, the same choice between specific MT numbers and a lumped MT5 representation can be made. This time however, there is no MT2 (elastic scattering). Similar to charged particles, we generally used the lumped MT5 representation for applied calculations A full, explicit MT description is also possible with TEFAL, but the processing route (by NJOY) is not entirely tested in that case.

4.1.4 MF4: Angular distributions of secondary particles

The versatility of MF6 (explained below) for the storage of almost any secondary distribution entails that one *may* choose to use MF4 for the neutron elastic scattering distribution only, while all other secondary angular distributions are stored in MF6. For (in)elastic scattering at incident energies below 20(60) MeV, Legendre coefficients are given on a sufficiently precise energy grid. They are a sum of calculated Legendre coefficients for compound nucleus and shape-elastic scattering. For

incident energies above 20(60) MeV, relative angular distributions are tabulated. TEFAL contains options to use either MF4 or MF6 for inelastic (MT51-90) or non-elastic (MT600-) scattering to discrete states. The choice between either MF4 or MF6 is often correlated with the choices for other secondary data (such as gamma production and covariance data), see Section 4.3.

4.1.5   MF5: Energy distributions of secondary particles

For modern evaluations, MF5 has almost completely been replaced by MF6, since the latter can take into account coupled energy-angle distributions. The only reason to still use MF5 is for the very important fission neutron spectra. Indeed, we use MF5/MT18 for this. The fission neutron spectrum may be produced by the TANES code [2]. If we adopt the fission neutron spectra from other libraries, we obviously adopt all associated ENDF-6 parameters as well.

> **Sample case 4.4** **20 MeV neutron general purpose file for ^{232}Th**
> The following *talys.inp* is used:
>
> ```
> #
> # n-Th232-fis
> #
> # General
> #
> projectile n
> element    Th
> mass       232
> ltarget    000
> energy     energies
> maxlevelstar    30
> partable y
> bins 40
> endf y
> #
> # do not use best parameters from database
> #
> best n
> #
> # set multi-preequilibrium switch lower for actinides
> #
> multipreeq 6.
> #
> # output of extra channels
> #
> channels y
> filechannels y
> #
> # reduce output for activation-only calculation
> #
> maxrot 2
> ```

```
strength 9
strengthm1 3
ngfit y
upbend y
ldmodel 5
fismodel 5
fispartdamp y
hbstate n
class2 n
ecissave y
eciscalc y
inccalc y
riplrisk y
#
# Current variables of TASMAN Run:  2509
#
ctable         90 233    1.35146 1
ptable         90 233 -1.94808E+00 1
ctable         90 233 -9.41013E-01 2
ptable         90 233    1.01594 2
ctable         90 233    3.16960 3
ptable         90 233 -1.14439E+00 3
betafiscor     90 233    1.04349
vfiscor        90 233    0.71170
ctable         90 232    0.32630 1
ptable         90 232    2.77492 1
ctable         90 232    8.34473 2
ptable         90 232 -6.59883E+00 2
ctable         90 232    0.69898 3
ptable         90 232    0.75241 3
betafiscor     90 232    0.50505
vfiscor        90 232    0.84379
ctable         90 231  5.77646E-02 1
ptable         90 231 -2.67866E+00 1
ctable         90 231 -3.61946E+00 2
ptable         90 231 -2.25936E+00 2
ctable         90 231 -2.85851E+00 3
ptable         90 231    2.66753 3
betafiscor     90 231    1.58614
vfiscor        90 231    1.62104
ctable         90 230 -3.18402E+00 1
ptable         90 230 -4.20179E+00 1
ctable         90 230    1.13153 2
ptable         90 230 -5.43220E-01 2
ctable         90 230    1.01315 3
```

```
ptable          90 230 -2.80603E+00 3
betafiscor      90 230    1.66138
vfiscor         90 230    1.71450
```

with which we run
talys < talys.inp > talys.out

For this sample case, we introduce some data from other libraries. The following TEFAL
input file is used

```
#
# Adoption of data from other libraries
#
adopt 1 452 n-Th232.endfb8.1
adopt 2 151 n-Th232.endfb8.1
adopt 5 18 n-Th232.jeff3.3
```

with which we run
tefal < tefal.inp > tefal.out

4.1.6 MF6: Product yields and energy-angle distributions

In MF6 we store all secondary distributions and relative particle and photon yields. The following
data can be included:
   - Angular distributions to discrete states for (n,n') (MT51-90), (n,p) (MT600-640), ... (n,α)
     (MT800-840), if they are not already included in MF4.
   - Double-differential spectra for exclusive channels (all MT-numbers for continuum channels)
     and recoil data.
   - Exclusive gamma yields for discrete states and continuum (all MT-numbers) if they are not
     stored in MF12,14 and 15.
   - Residual production yields (E > 20(60) MeV, MT5)
   - Total particle multiplicity, for (n,xn), (n,xp), ..., (n,xα) (E > 20(60) MeV, MT5)
   - Total particle energy and double-differential spectra (E > 20(60) MeV, MT5)

If MF4 is not already used for this, the angular distribution for inelastic scattering to each discrete
state may be given with Legendre coefficients up to 20(60) MeV. Next, for each discrete state the
exclusive yields for all the discrete gamma rays that originate from all other levels may be given.
Similarly, the angular distribution and gamma rays for the (n,p) etc. reactions to discrete levels may
be stored.

For continuum channels like (n,2n), etc., on a sufficiently dense incident energy grid the
secondary energy-angle distributions for each ejectile are specified by means of the relative emission
spectra and the parameters for the Kalbach systematics for angular distributions [11]. Next, if
MF12,14 and 15 are already not used, the photon yield is tabulated as a function of incident energy.
For each incident energy, the photon production is given for all discrete gamma lines present
in the final nucleus. A continuum photon distribution is added to this. We assume isotropy for
all produced gamma rays. Note that we thus in principle do not need MF12-15 for the photon
production that accompanies each reaction, although we have included the option to do that using
the **capt6, disc6** and **part6** keywords. As a final subsection, recoil data are given.

For energies above 20(60) MeV, MT5 may contain the production yields of particles and residual products. It also contains the secondary energy-angle distributions for all particles and photons. First, the yields for neutrons are given for the whole energy range. Next, on a secondary energy grid the relative emission spectra are given together with the parameters for the Kalbach systematics for angular distributions. Inelastic scattering cross sections for discrete states have been broadened and are added to the continuum spectra. This procedure is repeated for emitted protons, deuterons, tritons, Helium-3, alpha particles and photons. Finally, the residual production yields are given per final product and, if appropriate, separated for ground state and isomers. All these relative yields and distributions can be multiplied with the cross sections given in MF3/MT5 to get the production cross sections, single- and double-differential cross sections. In the subsections per residual product, the recoils are also given.

Charged-particle data

For incident charged particles, in MF6/MT2 the relative angular distributions for the nuclear and Coulomb-nuclear interference terms of elastic scattering are tabulated on an angular grid. Next, in MT5 the production yields of particles and residual products are stored, similar to neutrons but now for all energies, i.e. also below 20(60) MeV. The last paragraph of the section above for neutrons applies here too.

Sample case 4.5 60 MeV alpha activation file for ^{38}Ar

This sample case concerns a high-energy alpha activation library in ENDF-6 format. The following *talys.inp* is used:

```
#
# General
#
projectile a
element    ar
mass        38
energy     energies
endf y
#
# Precision
#
bins  40
popeps 1.e-12
transeps 1.e-20
transpower 15
xseps 1.e-20
#
# Specific
#
maxchannel 8
isomer 0.1
outgamdis n
outspectra n
```

```
outgamdis n
outangle n
outdiscrete n
ddxmode 0
```

    with which we run
    talys < talys.inp > talys.out

    The following TEFAL input file is used

```
#
# General
#
gpf n
high y
identifier ACF-2023
```

    with which we run
    tefal < tefal.inp > tefal.out

    and a library 'a-Ar038.acf' is produced.   ■

Photonuclear data

For incident photons, we usually take the lumped MF6/MT5 presentation, and discard angular
information. Complete energy spectra and residual cross sections are provided however.

Sample case 4.6 60 MeV gamma general purpose file for ^{64}Zn

This sample case concerns a high-energy photon data library, i.e. up to an energy of 60 MeV.
Again, no attempt was made to adjust the TALYS results to experimental data. This is a so
called "blind" data library. The following *talys.inp* is used:

```
#
# General
#
projectile g
element    zn
mass        64
energy     energies
endf y
#
# Precision
#
bins  50
popeps 1.e-12
transeps 1.e-20
transpower 15
xseps 1.e-20
```

```
#
# Specific
#
outgamdis n
```

with which we run
talys < talys.inp > talys.out

The following TEFAL input file is used

```
#
# General
#
renorm y
identifier LIB-2023
```

with which we run
tefal < tefal.inp > tefal.out

4.1.7 MF8/9/10: Production of radioactive nuclides

For reactions to nuclides with isomers, MF8 designates where the information for isomeric versus ground state production can be found. On the basis of the pointer set in MF8, isomeric production data are put in either MF9 or MF10. If the reaction channel has no threshold or has low energy resonances (such as (n,γ), (n,α), etc. with $Q > 0$), the branching ratios are put in MF9, which can then be combined with the cross sections in MF3 to create the final isomeric cross sections. For threshold reactions, the cross sections are stored directly in MF10, see also Ref. [12] for more details on these choices. By default, TALYS (and thus TEFAL also) treats final states with a lifetime that exceeds 1 second as isomer, but this can be set to another value in the TALYS input.

4.1.8 MF12/14/15: Photon yields and secondary distributions

If MF6 is not already used for this, MF12 can be used to store the photon production multiplicities or transition probability arrays. The latter is a simple representation in which the branching ratios for discrete levels are written to the data file, after which a processing code can combine this with the partial cross sections in MF3. We generally use this for discrete level reactions (MT51, etc.) Alternatively, the calculate relative photon yields can be given for partial cross sections. These result from the ratio of the photon production cross section and the (MF3) cross section. Total gamma ray yields and yields per discrete transition can be given.

As for photon angular distributions (MF14), we generally assume that they are isotropic, even though this is generally not true. There are a few reasons for taking isotropy: TALYS can currently not produce photon angular distributions and the applied relevance is, as far as we know, not very large.

If not already stored in MF6, continuum photon spectra can be given in MF15 for partial cross sections other than those to discrete levels.

4.2   Covariance data

The representation of uncertainty, or more general, covariance data in the ENDF-6 format is both limited and complex. Nevertheless, we generally try to incorporate a large amount of covariance data in our library. Even though we can apply this for any type of library, we outline this for incident neutrons only. This section is only relevant if the TASMAN code [2], to produce covariance data, is also installed.

4.2.1   MF31: Covariance data of number of fission neutrons

The covariance data for the number of fission neutrons are provided by the TAFIS code[2]. On the basis of rather simple assumptions a full covariance file for the total nubar is delivered.

4.2.2   MF32: Covariance data of resonance parameters

In MF32, we store the covariance data of resonance parameters, considering variations in the resonance energy and the neutron, radiative and fission widths. The uncertainties of these parameters are mainly based on the Atlas of Neutron Resonances [6], although other sources are used as well. For each isotope, the bound level resonance parameters, scattering radius and uncertainties have been adjusted to match the microscopic uncertainties (thermal elastic and capture cross sections as well as the capture integral), as given in the Atlas, or as extracted from evaluated libraries. For parameter correlation between Γ_n and Γ_γ, no long-range correlation is considered for the time being. As short-range correlation (between parameters of the same resonance), the method described in Ref. [10] is used. Uncertainties on cross sections have been checked and are partially presented in Refs. [13] and [14]. It should be noted that until recently the scattering radius could not be varied in the existing format for MF-32, (which would underestimate the elastic and total cross section uncertainties between resonances) however we have added its uncertainty in a vacant field in the header of each subsection. This is now part of the official ENDF-6 format. The covariance data of MF32 are all produced by the TARES code[3], although we also have the flexibility to read in data from existing libraries. Covariance data are given for both MF32 and MF33.

4.2.3   MF33: Cross section covariance data

In MF33, we store the covariance data of most, but not all, reaction channels that are given in MF3. All covariance data are generated with the TASMAN code, which generates TALYS runs using a Monte Carlo parameter sampling method. In principle, for each MT-number, the stored information may consist of:

1. Covariance matrix element for MT_1, E_1 and MT_1, E_1 (variances)
2. Covariance matrix element for MT_1, E_1 and MT_1, E_2 (correlations for the same reaction channel between different energies)
3. Covariance matrix element for MT_1, E_1 and MT_2, E_1 (correlations between different reaction channels for the same energy)
4. Covariance matrix element for MT_1, E_1 and MT_2, E_2 (correlations between different reaction channels for different energies)

but the latter completeness of inter-channel correlations is only used for very important channels. Classes 1 and 2 are covered by NI-type subsubsections with the flag LB=5, followed by an obligatory LB=8 section which contains the cross section variances multiplied by 1.e-3 (a suggestion taken over from S. Tagesen and used, for example, in the JEFF-3.0 Fe-56 file). These are the covariance data TEFAL writes by default. Classes 3 and 4 can also be covered by the flag LB=6 to account for

the different energy grids that two correlated MT-sections may have. Since the total correlation matrix is fully symmetric, we only need to include the correlation elements between different MT-numbers once, and we do that in the subsection with the lowest of the two MT-numbers. Usually, we include covariance information for all the total cross sections, the most important lumped partial cross sections and a few individual inelastic cross sections per level (MT51-54). We generally do not include covariance data for MT-numbers 600 and higher.

4.2.4 MF34: Covariance data for angular distributions

In MF34, we store the covariance data of the angular distributions that are given in MF4. All covariance data are generated with the TASMAN code, which generates TALYS runs using a Monte Carlo parameter method. We generally use MF34 only for elastic scattering (MT2), in which case covariance data are given for the first 6 Legendre coefficients. Both intra- and inter-correlations of the various Legendre coefficients are given. As in MF33, the LB5 representation is used.

4.2.5 MF35: Covariance data for energy distributions

The covariance data for fission neutron spectra are provided by the TANES code[2]. The contents of MF35 are covariance data between different outgoing energies of the neutron spectra.

4.2.6 MF40: Cross section production and isomer covariance data

In MF40, we store the covariance data for isomeric production, i.e. the covariance data belonging to MF10.

4.3 Preferred options for neutron libraries

So far, we explained all the ENDF-6 formatting options which are available in TEFAL. We go one step further now and discuss which of these possibilities could be used to create the "best" possible ENDF-6 file. For various types of quantities (MF numbers), more than one option is available, and these options can all be steered by a combination of TEFAL keywords. One may now ask why this is necessary. Isn't it possible to make a "best" ENDF-6 data file, in terms of ENDF-6 structure? And why should that structure differ from isotope to isotope? The latter question we may answer directly, and indeed, we see no reason to deviate from one ENDF-6 template, once its success is assessed. Still, the term "best" is subjective, and time dependent, since new insights in processing and integral validation may suggest changes in the preferred procedures in the future. The following choices will probably be under discussion for some time to come:

1. **Abrupt switch of MF3 representation at 20(60) MeV.** The classical procedure is to store data in specific MT numbers only up to 20(60) MeV, and use MT5 for energies above 20(60) MeV, while putting the values to zero in the other MT numbers. An alternative approach is to store data in specific MT numbers up to e.g. 200 MeV and use MT5 only for data which are not represented in other MT numbers. TEFAL provides both options, but we generally take the abrupt switch as default. Note however that an advantage of the other method is that cross section covariance data can be given up to 200 MeV instead of 20(60) MeV. A disadvantage is that all MT5 information such as residual production cross sections and cumulated spectra, need to be corrected for the data stored in other MT numbers. In TENDL, a switch at 30 MeV is used.

2. **Use all MT numbers or only the most important ones**. This is strongly related to the previous point. If one is using MT5 for the remaining cross sections anyway, one might also

include various unimportant reaction channels in it, even though special MT numbers exist for them. Since we use the abrupt switch as default, we can easily take all open channels up to 20(60) MeV into account, without producing an unnecessarily large file.

3. **Storage of discrete level data in MF6 or MF4 and 12**. Since MF6 is very versatile to store all kinds of secondary data, other MF numbers like MF4 or MF12 are, in principle, not necessary. However, users often want to have their data separated, for easier retrieval or processing. Therefore, we generally use MF4/MT51, etc. for inelastic angular distributions instead of MF6/MT51, etc. This has the additional advantage that one may provide covariance data in MF34/MT51, etc. for inelastic scattering angular distributions, something which is not possible for data stored in MF6. Once we have chosen for MF4/MT51, etc. it is also more consistent to store the gamma production data for discrete levels in MF12.

4. **Storage of photon production data in MF6 for partial, continuum channels.** For channels like (n,2n) it is on the other hand more convenient to give, besides double-differential spectra, photon production in MF6 instead of MF12 and MF15.

4.4   The EAF format

In principle, all cross section data can be represented, without information loss, in the ENDF-6 format. For the European Activation File [15] however, for historical reasons the so-called EAF format is used, which enables to represent all possible activation data using MF3 only, without resorting to MF8-10 for information on isomers. No other secondary information, i.e. MF4-15, is included. The activation code FISPACT-I relies completely on nuclear data in EAF format, and we have created an option in TEFAL to produce complete EAF activation files, even though we believe it is no longer necessary to maintain a separate activation library and that all "best" cross section values should be present in one general purpose library. An EAF file is supposed to be complete in terms of partial cross sections (i.e. all MT numbers should be included if the cross section is non-zero). The only rule for adoption in EAF is that the residual nucleus should not be in the same state as the target nucleus. This means that MT1,2,3,4,51-91 are not included, unless there is inelastic scattering to an isomer in which case this information is given in MT4. An "advantage" of an activation file is that there are no sum rules for the partial cross sections to be obeyed. The whole EAF library consists of a sequence of reaction blocks, one for each MT number. EAF libraries can be, and have been, made for all kinds of incident particles. With the release of the activation code FISPACT-II, the EAF format is expected to disappear.

4.4.1   MF3: Reaction cross sections

There are two important differences between the EAF and the ENDF-6 format, and they both concern the necessity to store all data in MF3:

- Isomeric data are stored in derived MT numbers, which are defined relative to the standard MT numbers, with MT+300 for production of the first isomer and MT+600 for the second isomer.
- To accommodate an extension up to 60 MeV, new MT numbers had to be assigned to various partial channels, which were not required for data files up to 20 MeV. These new MT numbers run from 151 to 200, and have become part of the official ENDF-6 format in 2010. It was checked with TALYS that the extended set of partial cross sections basically exhausts the reaction cross section below 60 MeV.

Besides these main deviations, other particular features of the EAF format are an extra comment line, the isomeric flag at the head of the file (where 99 designates the total, 0 the ground state and

isomeric state numbers are used for isomeric reactions), and the use of the temperature on the next line (consistently set to 0.). An example of a MF3 section of an EAF file is:

```
CO- 59N,NA              TALYS-2.0                               2759 3 22
 TALYS-2.0 Co59(n,na)Mn55 cross section                         2759 3 22
 2.705900+4 5.842693+1          0         99          0         02759 3 22
 0.000000+0-6.942208+6          0          0          1         442759 3 22
         44          2                                           2759 3 22
 7.061026+6 0.000000+0 9.000000+6 9.38343-14 9.500000+6 1.53228-102759 3 22
 1.000000+7 1.975079-8 1.050000+7 6.983146-7 1.100000+7 2.579987-62759 3 22
 1.150000+7 6.015733-6 1.200000+7 1.627379-5 1.250000+7 5.839929-52759 3 22
 1.300000+7 2.171970-4 1.350000+7 6.700209-4 1.400000+7 1.625576-32759 3 22
 1.450000+7 3.108140-3 1.500000+7 5.943940-3 1.600000+7 1.348706-22759 3 22
 1.700000+7 2.330049-2 1.800000+7 3.368735-2 1.900000+7 4.389603-22759 3 22
 2.000000+7 5.268588-2 2.100000+7 5.919127-2 2.200000+7 6.610421-22759 3 22
 2.300000+7 7.076757-2 2.400000+7 7.439464-2 2.500000+7 7.651939-22759 3 22
 2.600000+7 7.687765-2 2.700000+7 7.478991-2 2.800000+7 7.219817-22759 3 22
 2.900000+7 6.765909-2 3.000000+7 6.234970-2 3.200000+7 5.318324-22759 3 22
 3.400000+7 4.458247-2 3.600000+7 3.851828-2 3.800000+7 3.238804-22759 3 22
 4.000000+7 2.751206-2 4.200000+7 2.401153-2 4.400000+7 1.984092-22759 3 22
 4.600000+7 1.785219-2 4.800000+7 1.443929-2 5.000000+7 1.279484-22759 3 22
 5.200000+7 1.088498-2 5.400000+7 9.076456-3 5.600000+7 8.304118-32759 3 22
 5.800000+7 7.466814-3 6.000000+7 6.021678-3                    2759 3 22
                                                                1532 3  0
```

4.4.2 MF33: Cross section variances

For uncertainty calculations, the activation code FISPACT-I can currently only handle variance data, i.e. cross-energy and cross-channel correlations can not be taken into account in the activation calculations. Therefore, special EAF variance files can be produced with TEFAL provided, again, that the covariance generator TASMAN and the nuclear model code TALYS have been run first. The uncertainty data are given on a somewhat coarser energy grid than the cross sections, and are given as the relative variance, i.e. the square of the relative uncertainty. An example of a variance file is:

```
P - 32N,NA              TALYS-1.2                               153233 22   0
 1.503200+4 3.169924+1          0          0          0         1153233 22   0
 0.000000+0 0.000000+0          0         22          0         1153233 22   0
 0.000000+0 0.000000+0          0          1         22         11153233 22   0
 0.000000+0 0.000000+0 1.019140+7 0.000000+0 1.400000+7 6.948126-2153233 22   0
 1.800000+7 4.506280-2 2.200000+7 3.930505-2 2.600000+7 3.579096-2153233 22   0
 3.000000+7 3.744534-2 3.800000+7 4.460122-2 4.600000+7 3.690779-2153233 22   0
 5.400000+7 3.257014-2 6.000000+7 6.402975-2                    153233 22   0
                                                                153233  0   0
```

For example, the standard deviation of this cross section at 60 MeV is $\sqrt{(0.06402975)} = 0.25304$ or 25.304 %.

> **Sample case 4.7 60 MeV neutron EAF activation file for ^{59}Co**
> This sample case concerns a high-energy neutron activation library in EAF format. Files like this are adopted in the EAF library for activation/transmutation calculations. The following TALYS input file is used:

```
#
# General
#
projectile n
element    co
mass        59
energy      energies
endf y
#
# Precision
#
bins  40
popeps 1.e-12
transeps 1.e-20
transpower 15
xseps 1.e-20
#
# Specific
#
outgamdis n
outspectra n
outgamdis n
outangle n
outdiscrete n
ddxmode 0
maxchannel 8
isomer 0.1
```

with which we run

talys < **talys.inp** > **talys.out**

The following TEFAL input file is used

```
#
# General
#
gpf n
eaf y
high y
```

with which we run

tefal < **tefal.inp** > **tefal.out**

Note that this time the produced nuclear data file automatically got the extension '.eaf', *n-Co059.eaf*. ∎

5. Reference Guide

In this part, all TEFAL keywords will be described, one per page. The description of each keyword is as follows:

- Name of the keyword
- Explanation
- Examples
- Range of allowed values
- Default value
- Comments (optional), when we feel that some extra warnings or explanation for proper use is appropriate.

In each section, the keywords are roughly ordered by importance, rather than alphabetically. This is rather subjective of course, but it may make this part a bit more readable. Hence, it could be that the keywords near the end of certain Chapters are seldom used. In principle, all keywords may be referred to in the other parts of this tutorial.

5.1 Type of data library

The highest level of input is formed by the keywords that determine the type of library that is produced, such as e.g. a general purpose and/or activation library.

gpf

Flag for the creation of a complete ENDF-6 general purpose file.

Examples

gpf n
gpf y

Range

y or **n**

Default

gpf y

eaf

Flag for the creation of an EAF activation file.

Examples

> **eaf n**
> **eaf y**

Range

y or **n**

Default

eaf n

endfdetail

Flag to use specific MT numbers per reaction channel. With **endfdetail**, the corresponding value
read from the TALYS output file *endf.inf* can be overruled from **y** to **n**, i.e. even if detailed reaction
channel information was provided by TALYS, you may now choose to use a lumped presentation
using MT5. Of course, if the corresponding value in *endf.inf* is **n**, then the detailed information was
not produced by TALYS, and **endfdetail** can no longer be set to **y**. If you want that, a TALYS run
with keyword **endfdetail y** (the TALYS default), should be performed first.

Examples

> **endfdetail n**
> **endfdetail y**

Range

y or **n**

Default

The value of **endfdetail** is adopted from the TALYS output file *tefal.inf*.

endffile

The name of the final ENDF-6 file.

Examples

endffile co59.bviii

Range

endffile can be any filename, except the name of the TEFAL input file.

Default

The produced data library has a name containing the isotope and projectile under consideration and as extension '.gpf', '.acf', or '.eaf', depending of the type of data library, e.g. *n-Ge072.gpf*.

high

Flag for inclusion of data in the high energy lumped format, usually above 20(60) MeV, but more generally above the energy specified by **Eswitch**. Enabling this keyword means that the data is stored more implicitly using MT5 rather than in explicit MT sections at high energies.

Examples

high n
high y

Range

y or **n**

Default

high y

breakup

Flag to include special format for deuteron break-up double-differential cross sections, to enable Patrick Sauvan's extension to NJOY and MCNP.

Examples

> **breakup n**
> **breakup y**

Range

y or **n**

Default

breakup n

clean

Flag to clean up MF3,4, 6, 9 and 10. Many actions may be required by TEFAL to construct a data library: linearization, adoption from other libraries, taking care of the overlap with the resonance range (i.e. setting cross sections to zero) and adopting a huge amount of TALYS results, some of them small or zero. To make sure we get a "clean" MF3 we do some final checking after all the arrays are filled and, if needed, take actions if necessary, such as removing unnecessary zero values or removing more than 2 points with equal values. All cleaning actions are listed in the output file *tefal.clean*.

Examples

clean n
clean y

Range

y or **n**

Default

clean y

5.2   Limits, switches and tolerances

NMTmax

Maximum number of MT numbers.

Examples

NMTmax 100

Range

$3 \leq$ **NMTmax** $\leq$ **1000**

Default

NMTmax 400

Eswitch

Energy value above which the ENDF-6 representation switches from specific MT numbers to a lumped presentation using MT5.

Examples

Eswitch 30.
Eswitch 0. (only lumped cross sections)
Eswitch 200. (use specific MT numbers up to 200 MeV)

Range

$0. \leq$ **Eswitch** $\leq$ **300.**

Default

Eswitch 0. if no detailed MT information is required (i.e. if **endfdetail n** is set), and **Eswitch 30.** if detailed information is required for energies below **Eswitch** (i.e. if **endfdetail y** is set, usually for incident neutrons).

Eswitch4

Energy value above which the ENDF-6 representation for angular distributions switches from Legendre coefficients to tabulated angular distributions.

Examples

Eswitch4 30.
Eswitch4 0.

Range

$0. \leq$ **Eswitch4** $\leq 300.$

Default

Eswitch4 0. if no detailed MT information is required (if **endfdetail n** is set), and **Eswitch4 50.** if detailed information is required for energies below **Eswitch4** (if **endfdetail y** is set, usually for incident neutrons).

cuteps

Energy shift at MT5 cutoff energy (in eV).

Examples

cuteps 10.
cuteps 0.

Range

$0. \leq$ **cuteps** $\leq$ **100. eV**

Default

cuteps 0.

disclim

Limit for creating a specific MT number for a discrete level cross section. If the maximum cross section for the highest discrete level MT numbers is below **disclim**, the cross section is added to MT91, while the discrete level MT numbers are not used. In other words, we scan the discrete level excitation functions from the 40th level (MT90) down to the first (MT51), as soon as the maximum cross section is above **disclim**, we know the highest discrete level MT number. This circumvents the use of many unimportant MT numbers.

Examples

> **disclim 5.**
> **disclim 1.e-6**

Range

$0. \leq$ **disclim** $\leq$ **10000.**

Default

disclim 10.

maxrp

Maximum number of residual products that are stored.

Examples

maxrp 80

Range

$0 \leq$ **maxrp** $\leq$ **numrp**, where **numrp** is specified in *tefal.cmb*.

Default

maxrp 100

5.3 Specific structure of the data file

The world has not yet agreed on a unique way to store data in an ENDF-6 data file, so we must include some flexibility for this in TEFAL. If the defaults are used for the keywords in this section, our so-called "preferred" procedures outlined in chapter 4 will be applied. Deviations are possible with the keywords below.

mtall

Flag to include all defined MT numbers from the ENDF manual, see tables 4.1-4.1.3, rather than only the most important ones. If this flag is disabled, only MT1-5,16-22,28,37,38,51-91,102-107 will be used and the remaining cross sections will be added and stored in MT5.

Examples

    mtall n
    mtall y

Range

y or **n**

Default

mtall y

mtextra

Flag to include extra MT numbers from MT151 up to MT200. These MT numbers were approved as official ENDF format at the CSEWG meeting of 2010.

Examples

mtextra n
mtextra y

Range

y or **n**

Default

mtextra n. If **high y** and **eaf y** then **mtextra y** is forced.

exclude

Flag to exclude specific MT numbers which have been included by other, more global, keywords such as **mtall**. For example, to avoid "contamination" of the total cross section in MT1 with a very small low energy (n, α) cross section for actinides, we may want to disable it.

Examples

> **exclude 107**
> **exclude 3**

Range

$1 \leq$ **exclude** $\leq$ **849**

Default

include

Flag to include specific MT numbers which have been excluded by other, more global, keywords such as **mtall**.

Examples

      include 11

Range

$1 \leq \text{include} \leq 849$

Default

nomf

Flag to exclude an entire MF. This is mostly for testing purposes, or to temporarily solve e.g. processing problems.

Examples

nomf 10
nomf 33

Range

$1 \leq \mathbf{nomf} \leq 40$

Default

capt6

Flag to store photon production data for the neutron capture channel (MT102) in MF6 instead of MF12-15. Often, experimental gamma lines from thermal capture may be available, and then it may be more convenient to store the data in MF12.

Examples

capt6 n
capt6 y

Range

y or **n**

Default

capt6 y

disc6

Flag to store all secondary data for discrete level reactions (MT51-90) in MF6 instead of MF4 (angular distributions), MF12 and MF14 (photon production).

Examples

disc6 n
disc6 y

Range

y or **n**

Default

disc6 n for incident neutrons, **disc6 y** otherwise.

part6

Flag to store all secondary data for partial reactions ((n,2n), (n,p), etc.) in MF6 instead of MF4 (angular distributions), 12, 14 and 15 (photon production).

Examples

part6 n
part6 y

Range

y or **n**

Default

part6 y

tabddx

Flag to give explicit double-differential energy-angle distributions in MF6 instead of Kalbach systematics.

Examples

tabddx n
tabddx y

Range

y or **n**

Default

tabddx n

ngn

Flag to include (n,γ n) data explicitly in MT5, instead of adding it to the continuum (n,n') cross section (MT91). Note that if **ngn n**, a small error is necessarily made since MT91 must start at a thresh

Examples

    ngn n
    ngn y

Range

y or **n**

Default

ngn n

rp6

Flag to store (high-energy) residual production cross sections in MF6.

Examples

rp6 n
rp6 y

Range

y or **n**

Default

rp6 y

rp10

Flag to store (high-energy) residual production cross sections in MF10.

Examples

rp10 n
rp10 y

Range

y or **n**

Default

rp10 y

addlow

Flag to add low-energy exothermic reactions, other than (n,γ), such as (n,p) and (n,α) to the total cross section, to reactions which are not included in MF2.

Examples

addlow n
addlow y

Range

y or **n**

Default

addlow y

partialn

Flag to include or exclude cross sections and secondary distributions for (proj,n') reactions to discrete levels and continuum (MT51-90). If disabled, only MT4 will be used.

Examples

partialn n
partialn y

Range

y or **n**

Default

partialn y for incident photons or neutrons, otherwise **partialn n**

partialp

Flag to include or exclude cross sections and secondary distributions for (proj,p) reactions to discrete levels and continuum (MT600-649). If disabled, only MT103 will be used.

Examples

partialp n
partialp y

Range

y or **n**

Default

partialp n

partiala

Flag to include or exclude cross sections and secondary distributions for (proj,a) reactions to discrete levels and continuum (MT800-849). If disabled, only MT107 will be used.

Examples

partiala n
partiala y

Range

y or **n**

Default

partiala n

partiald

Flag to include or exclude cross sections and secondary distributions for (proj,d) reactions to discrete levels and continuum (MT650-699). If disabled, only MT104 will be used.

Examples

partiald n
partiald y

Range

y or **n**

Default

partiald n

partialt

Flag to include or exclude cross sections and secondary distributions for (proj,t) reactions to discrete levels and continuum (MT700-749). If disabled, only MT105 will be used.

Examples

partialt n
partialt y

Range

y or **n**

Default

partialt n

partialh

Flag to include or exclude cross sections and secondary distributions for (proj,h) reactions to discrete levels and continuum (MT750-799). If disabled, only MT106 will be used.

Examples

partialh n
partialh y

Range

y or **n**

Default

partialh n

gam13

Flag to store photon production data in MF13 (cross sections) instead of MF12 (yields).

Examples

gam13 n
gam13 y

Range

y or **n**

Default

gam13 n

fis10

Flag to put (subactinide) fission cross sections in MF10.

Examples

fis10 n
fis10 y

Range

y or **n**

Default

fis10 n

gamdiscrete

Flag to store photon production data per discrete level cross section (MT51..) instead of in the total of MT4.

Examples

gamdiscrete n
gamdiscrete y

Range

y or **n**

Default

gamdiscrete y

renorm

Flag to renormalize spectra to the cross sections. Even though this should already be taken care of as much as possible by TALYS, this action is included as an extra step to ensure unitarity.

Examples

renorm n
renorm y

Range

y or **n**

Default

renorm y

recoil

Flag to include recoil information.

Examples

recoil n
recoil y

Range

y or **n**

Default

recoil is read from the TALYS output file *endf.inf*. In other words, if *recoil y* was set in the TALYS input file, then this will automatically be used in TEFAL.

subfission

Flag to include subactinide fission.

Examples

> **subfission n**
> **subfission y**

Range

y or **n**

Default

subfission n

multichance

Flag to include multi (1st up to 4th) chance fission data, i.e. MT19-21,38.

Examples

multichance n
multichance y

Range

y or **n**

Default

multichance y

linenumbers

Flag to include linenumbers in the ENDF file.

Examples

linenumbers n
linenumbers y

Range

y or **n**

Default

linenumbers y

5.4 Use of specific data

There are various data for which TALYS is not yet appropriate, e.g. resonance data, or for which still better alternatives exist in other data sources. We have enabled the possibility to include such data through a few keywords.

adopt

Keyword to adopt parts of an existing ENDF-6 formatted file. On the input line, we read **adopt**, the MF number, optionally the MT number, the ENDF-6 file from which we read the data, and optionally the lower and the upper energy in eV. If the MT number is not specified, the keyword holds for the entire MF. If the energy range is not specified, the keyword holds for the entire energy range. The adopted data will overrule TALYS data for the specified MF-MT section and energy range.

Examples

adopt 1 452 fission.mt452.0000: the total average number of fission neutrons will be adopted from an ENDF-6 formatted file *fission.mt452.0000* which should be present in your working directory,

adopt 2 151 mf2.res: the resonance parameters will be adopted from an ENDF-6 formatted file *mf2.res* which should be present in your working directory,

adopt 2 151 n-Zr090.jeff3.3: the resonance parameters will be adopted from an ENDF-6 formatted file of JEFF-3.3. working directory,

adopt 3 1 n-Pd106.jeff3.3 1.e5 2.e6: the total cross section for Pd-106 in the energy range between 100 keV and 2 MeV will be adopted from the JEFF-3.3 library,

adopt 3 n-Fe056.endfb8.0: all cross sections (i.e. the entire MF3) for Fe-56 in the whole energy range will be adopted from the ENDF/B-VIII library,

adopt 4 2 n-Fe056.endfb8.0: the elastic scattering distribution for Fe-56 in the whole energy range will be adopted from the ENDF/B-VIII library,

adopt 5 18 fns.mf5: the fission neutron spectrum will be adopted from an ENDF-6 formatted file *fns.mf5* which should be present in your working directory,

adopt 12 102 n-Al027.endfb8.0: the neutron capture yield data for Al-27 will be adopted from the ENDF/B-VIII library,

adopt 32 151 mf2.res.mf32c: covariance data for the resonance parameters will be adopted from an ENDF-6 formatted file *mf2.res.mf32c* which should be present in your working directory.

Range

the file of **adopt** should exist either as a local file in your working directory or in the *libraries/* database. In the latter case, the filename extension of **adopt** should be equal to **cendl3.2**, **irdff2.0**, **tendl.2021 endfb8.0**, **jeff3.3**, **jendl4.0**, **eaf.2010**. Note that TEFAL automatically searches in *libraries/* Note also that the mass number in these files should be given in i3.3 format, as in *n-Fe056.endfb8.0*. The MF number should be between 1 and 40. The MT number should be between 1 and 849. The energy range should be between 10^{-5} and 2.10^8 eV.

Default

adopt is not used.

resonance

Flag to include resonance parameters from an external source (y) or use a skeleton MF2 with the potential scattering radius (n).

Examples

resonance n
resonance y

Range

y or **n**

Default

resonance y

background

Name of the file to be adopted for background cross sections in MF3/MT1,2,3,18,102, in case there is a background cross section to be added to the resonance parameters of MF2.

Examples

background n-Pu239.endfb8.0

Range

The **background** file should exist in either your working directory or in the *libraries/* database.

Default

if the file of **adopt 2 151** comes from one of the libraries in the libraries database, e.g. *n-Pu239.endfb8.0*, that same file is taken for **background** as default, and the keyword in the example above is not necessary. In other cases **background** does not have a default.

urrmode

The way to handle unresolved resonance parameters.

Examples

      urrmode 0: No URR
      urrmode 1: URR taken from TALYS
      urrmode 2: URR taken from existing data library

Range

$0 \leq$ **urrmode** ≤ 2

Default

urrmode 1 if set by TALYS and *tefal.inf*, **urrmode 2** otherwise. **urrmode 0** for $A \leq 20$.

urrenergy

Upper energy of the unresolved resonance range.

Examples

urrenergy 0.084

Range

$0. \leq$ **urrenergy** $\leq 1.$

Default

urrenergy 0.1

lssf

LSSF value to overrule that of the included resonance file. LSSF=0 means the URR cross section should be constructed from MF2, LSSF=1 means the URR cross section is given in MF3 while the MF2 parameters are just used for self-shielding.

Examples

lssf 1

Range

$0 \leq \text{lssf} \leq 1$

Default

lssf is not given, i.e. take the value of the adopted MF2 file.

urrcomp

Flag to include or exclude competing channels that may have overlap in energy with the URR.

Examples

  urrcomp 0: MT4 and other open channels are zero in the URR range
  urrcomp 1: MT4 is zero in the URR range
  urrcomp 2: all overlap allowed

Range

$0 \leq$ **urrcomp** ≤ 2

Default

urrcomp 1

5.5 Information for MF1

The MF1 part of an ENDF-6 file contains descriptive information, such as the author, name of institute, and text that describes the contents of the data files. A few keywords can be used for this.

author

Author of data file. This will appear in the header of MF1.

Examples

author J. Raynal

Range

author can be any name.

Default

author A.J. Koning.

lab

Lab (or institute) where the data file was produced. This will appear in the header of MF1.

Examples

lab CEA

Range

lab can be any name, but will be truncated to 11 characters.

Default

lab IAEA.

identifier

Name of library. This will appear in the header of MF1.

Examples

identifier JEFF-3.1

Range

identifier can be any name.

Default

identifier TENDL-2021

endftext

File with information text to be read for MF1.

Examples

endftext co59.txt

Range

endftext can be any filename.

Default

endftext is taken from the *aux/* directory, where default text files are stored, which depend on the type of projectile and type of library.

diffweight

Differential weight to be put in MF1. This is to track the specific weight of a random file when compared with experimental data.

Examples

diffweight 0.445234

Range

diffweight can be any real number.

Default

diffweight not used.

5.6 Covariance data

Covariance data can be included in the data file if a combination of the TASMAN and TALYS codes has been run first. After that, there are various options to include covariance data to a user-defined amount of complexity.

covariance

Flag to include covariance data.

Examples

> **covariance n**
> **covariance y**

Range

y or **n**

Default

covariance n

partialcov

Flag to include or exclude covariance data for (n,p), (n,d), (n,t), (n,h) and (n,α) reactions to discrete levels and continuum (MT600-849). If disabled, only covariance data for MT103-107 will be used.

Examples

partialcov n
partialcov y

Range

y or **n**

Default

partialcov n

covdiscrete

Number of discrete inelastic levels (MT51-90) with covariance data.

Examples

covdiscrete 4

Range

$0 \leq$ **covdiscrete** $\leq$ **40**

Default

covdiscrete 4

intercor

Flag to include or exclude inter-channel cross section correlations, i.e. correlations between different MT numbers.

Examples

intercor n
intercor y

Range

y or **n**

Default

intercor y

covrp

Flag to include or exclude covariances for residual production cross sections. This keyword is not yet active, but will become when processing codes are able to deal with this.

Examples

covrp n
covrp y

Range

y or **n**

Default

covrp n.

cross

Flag to run TASMAN for covariances or optimization of cross sections.

Examples

cross n
cross y

Range

y or **n**

Default

cross y

nocross

Specific MT numbers for which inter-channel cross section correlations are excluded, in addition to the default.

Examples

nocross 16
nocross 104

Range

$1 \leq$ **nocross** $\leq$ **849**

Default

Cross correlations are excluded for all MT-numbers except MT1,2,3,4,16,18,51,91,102,103,107.

Table 5.1: The keywords of TEFAL.

Keyword	Range	Default	Page
addlow	y,n	y	70
adopt	filename	no default	86
author	name	A.J. Koning	94
background	filename	file of **adopt 2 151**	88
breakup	y,n	n	48
capt6	y,n	y	63
clean	y,n	y	49
covariance	y,n	n	100
covdiscrete	0-40	4	102
covrp	y,n	n	104
cross	1-849	most important MT's	105
cuteps	0.-100.	0.	54
diffweight	real number	none	98
disc6	y,n	n for incident n, y otherwise	64
disclim	0.-10000.	10.	55
eaf	y,n	n	44
endfdetail	y,n	from *endf.inf*	45
endffile	filename	name of isotope	46
endftext	filename	from aux/ directory	97
Eswitch	0.-300.	30. for incident n,γ, 0 otherwise	52
Eswitch4	0.-300.	50. for incident n,γ, 0 otherwise	53
exclude	1-849	none	60
fis10	y,n	n	78
gam13	y,n	n	77
gamdiscrete	y,n	y	79
gpf	y,n	y	43
high	y,n	y	47
identifier	name	TENDL-2021	96
include	1-849	none	61
intercor	y,n	y	103

Continuation of **Table 5.1.**

Keyword	Range	Default	Page
lab	name	IAEA	95
linenumbers	y,n	y	84
lssf	0-1	none	91
maxrp	0-numrp	100	56
mtall	y,n	y	58
mtextra	y,n	n	59
multichance	y,n	y	83
ngn	y,n	n	67
NMTmax	3-1000	400	51
nocross	1-849	least important MT's	106
nomf	1-40	none	62
part6	y,n	y	65
partiala	y,n	n	73
partialcov	y,n	n	101
partiald	y,n	n	74
partialh	y,n	n	76
partialn	y,n	y	71
partialp	y,n	n	72
partialt	y,n	n	75
recoil	y,n	from *endf.inf*	81
renorm	y,n	y	80
resonance	y,n	y	87
rp10	y,n	y	69
rp6	y,n	y	68
subfission	y,n	n	82
tabddx	y,n	n	66
urrcomp	0-2	1	92
urrenergy	0.-1.	0.1 (100 keV)	90
urrmode	0-2	from *endf.inf*, 2 otherwise	89

6. Outlook and conclusions

This tutorial describes TEFAL, an ENDF-6 formatting code to translate the results of TALYS in combination with possible data from other sources, into nuclear data libraries. With the TALYS-TEFAL combination we can cover the whole path from basic nuclear reaction measurements and models to the creation of complete data libraries for nuclear applications. In the last few years, the TEFAL code has been used to create many nuclear data libraries. The main output of that can be found in the TENDL[2] library, which is a complete nuclear data library, i.e. for all isotopes, incident particles and energies, that now has evolved into a library that rivals with the major nuclear data libraries in the world. Also various files made with this system are now part part the JEFF-3.3 and ENDF/B-VIII libraries, while the final version of the European Activation File, EAF-2010, already heavily relied on the TALYS-TEFAL combination.

Although TEFAL is already quite extensive, robust and flexible, there are still minor additions that could be implemented. Also, we want to reach the state where "library cloning and extending" is automated and robust. Then, e.g. an ENDF/B-VIII, JENDL, or JEFF library could be read by TEFAL (and TALYS) after which TEFAL delivers the same "core evaluation" but extended with all data (high-energy data, angular distributions, spectra, gamma production, covariance data, etc.) that is not present in the original library. Looping over all nuclides would then produce a "ENDF/B-VIII++" or "JEFF4++" library. For this, it will be necessary to read in *any* part of an existing data library and to correct for this in the TALYS-based results, i.e. to make sure the sum rules are always obeyed. These, and other extensions, are still to be accomplished.

The final remark here is that the ENDF-6 format is archaic, error-prone, not keyword-driven, difficult to maintain but also present in basically all applied nuclear software that relies on nuclear reaction data. Modernization is underway by e.g. the FUDGE code which is now able to directly translate TALYS output files into the GNDS format, and this route will probably take over from the ENDF-6 formatting by TEFAL in the future.

Bibliography

[1] A.J. Koning, S. Hilaire, and S. Goriely. "TALYS: modeling of nuclear reactions". In: *European Physical Journal A* 59 (2023), p. 131.

[2] A.J. Koning et al. "TENDL: Complete Nuclear Data Library for innovative Nuclear Science and Technology". In: *Nuclear Data Sheets* 155 (2019), p. 1.

[3] J.-Ch. Sublet D. Rochman A.J. Koning. "A statistical analysis of evaluated neutron resonances with TARES for JEFF-3.3, JENDL-4.0, ENDF/B-VIII.0 and TENDL-2019". In: *Nuclear Data Sheets* 163 (2020), p. 163.

[4] A.J. Koning and D. Rochman. "Modern nuclear data evaluation with the TALYS code system". In: *Nuclear Data Sheets* 113 (2012), p. 2841.

[5] A. Trkov, M. Herman, and D.A. Brown. *ENDF-6 Formats Manual, Data Formats and Procedures for the Evaluated Nuclear Data Files ENDF/B-VI, ENDF/B-VII and ENDF/B-VIII*. CSEWG Document ENDF-102, Report BNL-203218-2018-INRE, SVN Commit: revision 215. 2012.

[6] S. F. Mughabghab. *Atlas of Neutron Resonances*. 6th ed. The Netherlands: Elsevier, 2018.

[7] MB Chadwick et al. "Cross-section evaluations to 150 MeV for accelerator-driven systems and implementation in MCNPX". In: *Nuclear Science and Engineering* 131.3 (1999), pp. 293–328.

[8] A.J. Koning. *Requirements for an evaluated nuclear data file for accelerator-based transmutation*. 1993.

[9] AJ Koning, A Hogenbirk, and O Bersillon. *High-energy nuclear data files: From ENDF-6 to NJOY to MCNP*. 1997.

[10]   D Rochman and AJ Koning. "Pb and Bi neutron data libraries with full covariance evaluation and improved integral tests". In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 589.1 (2008), pp. 85–108.

[11]   C. Kalbach. "Systematics of continuum angular distributions: Extensions to higher energies". In: *Phys. Rev. C* 37 (6 1988), pp. 2350–2370. DOI: 10.1103/PhysRevC.37.2350. URL: https://link.aps.org/doi/10.1103/PhysRevC.37.2350.

[12]   J-Ch Sublet et al. "The JEFF-3.0/A Neutron Activation File (New Features, Validation, and Usage". In: *AIP Conference Proceedings*. Vol. 769. 1. AIP. 2005, pp. 203–206.

[13]   Dimitri Rochman, Arjan J Koning, and Steven C van der Marck. "Uncertainties for criticality-safety benchmarks and keff distributions". In: *Annals of Nuclear Energy* 36.6 (2009), pp. 810–831.

[14]   Arjan J Koning and Dimitri Rochman. "Towards sustainable nuclear energy: Putting nuclear physics to work". In: *Annals of Nuclear Energy* 35.11 (2008), pp. 2024–2030.

[15]   J.-Ch. Sublet et al. *Activation File: EAF-2010 neutron-induced cross section library*. Tech. rep. EASY Documentation Series CCFE-R (10) 05. UKAEA, 2010.